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Change in Density of States in a Resonant Tunneling Structure due to a Scattering Center in the Well

by

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# Change in density of states in a resonant tunneling structure due to a scattering center in the well

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The change in density of states and transmission resonance energy shifts have been calculated for a double-barrier single-quantum-well heterostructure by placing a scattering center in the middle of the well and representing it by (1) a thin barrier of variable height and fixed width or (2) a delta-function potential of variable strength. It is found that the energies of the even resonance states shift towards the higher energies and states get broader as the height of the thin barrier increases. Similar behavior is observed for the delta-function potential as the strength of the delta-function potential increases. The peak value of the density of states versus energy plot are reduced for even resonance states due to the broadening of these states. The physical processes related with these behavior are discussed. Moreover, there are no changes in the odd resonance states because of the nature of their wave functions in the well region of the resonant tunneling structure.

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## INTRODUCTION

The progress of semiconductor fabrication technology, particularly the molecular beam epitaxy (MBE), has permitted the construction of structures and devices whose properties are dominated by quantum interference effects. Recently, very narrow potential barrier profiles have been produced in GaAs /  $Al_xGa_{1-x}As$  superlattices.<sup>1,2</sup> The intentional doping has been implemented by positioning Si donors and Be acceptors in precise numbers during the MBE growth of GaAs layers. This so-called sheet-doping (or delta-doping) technique. originally proposed by Wood et al.<sup>3</sup> has been applied in advanced semiconductor device techniques. The confinement of donors or acceptors to selectively doped  $GaAs /Al_xGa_{1-x}As$  heterostructures leads to high mobilities and to high two-dimensional carrier densities. Since the early studies by Chang, Tsu and Esaki<sup>4-6</sup> of resonant tunneling through quantum-well states and negative differential resistance in double barriers heterostructures, there have been numerous investigations of one-dimensional resonant tunneling structures (RTS) and quantum wells (QW). These RTS and QW are not only important in microdevices but their study involves a great deal of basic physics. Most of the theoretical investigations of the static properties of the RTS have been limited to the calculation of irausmission coefficients through the interfaces of the RTS. However, in recent years it has been realized that the study of the electronic density of states of RTS is equally important due to the applicability of RTS and QW in optical devices.7 It has also been noticed that the density of states provide a better representation of states in comparison with the transmission coefficients since there are some circumstances where transmission coefficients do not exist.

There have been different approaches to study the electronic density of states of RTS. For example, Bahdr and coworkers<sup>3</sup> calculated the local density of states by means of Green's functions. Their calculations were for the RTS where the two barriers are represented by two delta( $\delta$ )-function potentials, and later they included the finite width for the barriers in their calculations. The global density of states from the local density of states of Ref. 8 can be shown to be identically zero. Bloss<sup>9</sup> has calculated the wave function in the well region of the RTS under bias. He has shown that the integral value of the square of the wave function over the well region of the RTS and the density of states are correlated. Kim and Arnold<sup>10</sup> have also-performed some calculations for the local density of states using the nonequilibrium tunneling theory of Caroli et al<sup>11</sup> and the scattering-theoretic Green's-function technique with a simple Hamiltonian. However, none of these investigations have considered the effect of a scattering center on the density of states.

A model calculation of the electronic states of a superlattice of period a interleaved with a periodic array of  $\delta$ -function impurity centers has been reported by Beltram and Capasso<sup>12</sup>, who found that through a judicious choice of the width of the quantum well and location of the impurity, the width of the minibands could be controlled. Earlier, Stone and Lee <sup>13</sup> had considered the effect of inelastic scattering on tunneling resonances in one dimension.

Recently, we presented a simple technique to calculate the change in the global density of states of RTS. 14.15 The technique described in Refs. 14 and



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15 is suitable for calculating the global density of states for any potential profile within a box. This density was calculated for the RTS in the box and compared with the density of states of the empty box. We found that the states are piled up at the resonance energies and pushed away in the energy regions away from the resonance energies. A plot of the density of states versus energy shows a peak at the transmission resonance energies if the resonance is sharp. Otherwise the peak of this plot is shifted from the transmission resonance energy. A linear decrease in the resonance energy and broadening of the states as a function of bias voltage are observed. For an asymmetric RTS, the plots of transmission coefficients and the change in density of states have left-right symmetry with respect to the interchange of the two barriers of the RTS. This symmetry is broken in the case of an asymmetric RTS under bias.

In this paper, we have used an extra thin barrier or a  $\delta$ -function potential in the well to describe the perturbation potential of a scattering center and study its effect on the transmission and change in the global density of states. The corresponding changes in the bound states of the RTS are important in the interstate transition studies. It is found that the extra thin barrier and  $\delta$ -function potential in the middle of the well moves the even bound states up, while the odd states remains unchanged. The widths of the even states get broader as the thin barrier height increases or the strength of the  $\delta$ -function potential increases. The density of states for the energies of even states is reduced due to the broadening of the states.

### CALCULATIONAL TECHNIQUE

The method to calculate the transmission coefficients T(E) as function of electron energy E through a potential profile such as RTS are well described in the literatures. <sup>16,17</sup> To calculated the global density of states, the procedure laid out in Refs. 14 and 15 is followed here. For the sake of completeness, a brief description to calculate the density of states is given below. The local density of states is

$$N(E,x) = \sum_{j} \delta(E - E_j) |\Psi(x, E_j)|^2, \qquad (1)$$

where  $\Psi(x, E_j)$  and  $E_j$  are the eigenfunctions and eigenvalues, respectively. The global density of states obtained by integrating Eq. (1) will be identically zero.<sup>8</sup> Therefore, a different method to calculate the global density of states,

$$N(E) = \sum_{j} \delta(E - E_{j}),$$

has been adopted here. In this way, a change in the spacing of energy levels brought in by RTS contributes to the density of states without involving any particular spatial region. Let us consider a box of length L and walls extended to infinity. The eigenstates of this box,  $\frac{n\pi}{L}$  where n is an integer, are equally spaced in k-space, and the inverse of the spacing, which is the density of states, is constant for a given L and increases linearly with L. The spacing of eigenstates becomes disturbed by a small RTS in the box. This change in the spacing brought by the RTS has been calculated to find the change in the global density of states. The RTS in the box produces a phase change in the eigenfunction. The solution of the Schrödinger equation for an electron in a box extending from

0 to L is  $\sqrt{\frac{2}{L}}\sin(\frac{n\pi}{L}x)$ , and the solution for an electron in a box with the RTS is  $A\sin(\frac{n\pi}{L}+\phi)x$  with A as a normalization constant. Depending upon the the position of the RTS in the box, the phase difference,  $\phi$ , forms different patterns, where each pattern is called a subdensity.<sup>14</sup> The sum of changes contributed by all the subdensities gives the change in the global density of states due to the RTS.

A schematic illustration of the scructure considered here is given in Fig. 1. An RTS of a few hundred Å total width with an extra thin barrier or a  $\delta$ -function potential in the well region is placed in a box of length L. The value of L ranges from  $10^6$  to  $10^8$  Å depending upon the resolution needed for resonance states. The RTS is placed at a distance  $x_1$  from the left wall of the box. The two barriers of the RTS extend from  $x_1$  to  $x_1 + a_1$  and  $x_1 + a_1 + d$  to  $x_1 + a_1 + d + a_2$ , where d is the well width and  $a_1$  and  $a_2$  are widths of the left and right barriers. The heights of the barriers are  $V_L$  and  $V_R$ . A thin barrier of variable height and fixed width, b, ranging from  $x_1 + a_1 + \frac{d-b}{2}$  to  $x_1 + a_1 + \frac{d+b}{2}$  where  $b \ll d$ , or a  $\delta$ -function potential at  $x_1 + a_1 + c (\leq x_1 + a_1 + d)$ , in the well has been considered as an extra potential profile in the RTS. The eigenvalue condition, namely the vanishing of the wave function at x=L, can be given as

$$D(k) = A_4(k)\sin k(L - x_2) + B_4(k)\cos k(L - x_2) = 0,$$
 (2)

where  $x_2 = x_1 + a_1 + d + a_2$  and  $A_4(k)$  and  $B_4(k)$  are the amplitudes of the envelop wave function in the region from  $x = x_2$  to x=L. The amplitudes  $A_4(k)$  and  $B_4(k)$  can be calculated easily by requiring wave functions and their derivatives to be continuous across the interfaces of the RTS. Here  $k = \sqrt{\frac{2m^*E}{\hbar^2}}$  and  $m^*$  is the

effective mass of the electron. A constant value of  $m^*$  (=0.067 $m_*$ , with  $m_*$  as the electron mass) has been taken throughout the structure in our calculation for simplicity. For the case of a different effective mass, the derivative of the wave function divided by the effective mass of the region should be continuous instead of the derivative alone.  $^{18-20}$  The positions of the resonance states get lowered slightly, but the widths of the states broaden considerably for the case in which one considers different effective masses.  $^{21}$  So, in the calculation where a comparison with the experiment, especially the dwell time, is undertaken, the correct value of the effective masses of different materials should be considered.

The change in the density of states in k-space in comparison with a free box can be calculated as

$$\Delta N(k_n) = \frac{1}{\Delta k_n} - \frac{L}{n\pi},\tag{3a}$$

and hence,

$$\Delta N(E) = \Delta N(k) \frac{m^*}{\hbar^2 k}. \tag{3b}$$

Here  $\Delta k_n = k_n - k_{n-1}$  and  $k_n$  and  $k_{n-1}$  are calculated from Eqn. (2). As mentioned earlier,  $\Delta N(k)$  or  $\Delta N(E)$  should be calculated for all the subdensities and summed over all subdensities to give the change in global density of states.

#### RESULTS AND DISCUSSION

The structure under investigation is shown in Fig. 1 for an asymmetric RTS in a box. Parameters used in the calculation are as follows: for a symmetric RTS,  $a_1 = a_2 = 50$  Å, d=150 Å and  $V_L = V_R = 200$  meV, and for an asymmetric RTS,  $a_1 = a_2 = 50$  Å, d=150 Å,  $V_L = 200$  meV and  $V_R = 180$  meV. The position of the symmetric and asymmetric RTS is  $x_1 = \frac{L}{2}$ , at which two subdensities are formed.

For the parameters described above, there are three resonances at  $16.5\pm0.0434$ .  $64.87\pm0.540$  and  $140.76\pm3.72$  meV for the symmetric RTS, and  $16.33\pm0.0533$ .  $64.1\pm0.661$  and  $138.8\pm4.49$  meV for the asymmetric one. The escape times for these three resonance states,  $t_{es} = \frac{\hbar}{\delta E}$ , where  $\delta E$  is the width of the states, are 15.2, 1.22 and 0.177 ps for the symmetric RTS, and 12.3, 1.0 and 0.147 ps for the asymmetric one, respectively. It is clear that as the states move closer to the surface of the well, the escape times get smaller and smaller. An electron at the state deep inside the well takes more time to tunnel through the barriers than the one at the state closer to the surface of the well, which is a signature of the time-energy uncertainty relation.

On the left side of the Fig. 2, the results for transmission T(E) and change in density of states,  $\Delta N(E)$  for the symmetric (solid curves) and for the asymmetric RTS (dashed curves) with a thin barrier of 15 Å width and 10 meV height as an extra potential profile are shown in the first resonance energy range. For the sake of comparison, results without an extra potential profile (dotted for symmetric and dot-dashed for asymmetric RTS) are also plotted in Fig. 2. Corresponding results for a  $\delta$ -function potential ( 100 meV·Å strength in the middle of the well) as an extra potential profile are displayed on the right side of the Fig. 2. It is clear that the energy of the first resonance state shifts towards the higher energy for both the thin barrier and  $\delta$ -function potentials. As mentioned earlier, the width of the state which shifts towards the surface of the well should increase from the time-energy uncertainity relation. This behavior is not quite apparent from the Fig. 2 because of the narrowness of the state. The peak value of

 $\Delta N(E)$  is reduced in comparison with the peak value of  $\Delta N(E)$  for the RTS without an extra potential profile. However, T(E) attains the value of unity for the symmetric RTS and reduces to a definite value less than unity for the asymmetric one. The reason for the change in  $\Delta N(E)$  is that a quantity

$$\Delta N = \int dE \Delta N(E) \tag{4}$$

should have the value of unity for a single bound state. For  $\Delta N$  to be unity, a lower value of  $\Delta N(E)$  at the resonance energy makes it clearer that the width of the resonance has increased for a finite value of the thin barrier height and finite strength of the  $\delta$ -function potential. A further discussion of the quantity  $\Delta N$  is given later in the text. Although there is no direct correlation between the width and height of the thin barrier and the strength of the  $\delta$ -function potential, a correspondence between them can be derived from Fig. 2.

The results for the second resonance state are shown in Fig. 3. In this figure the change in resonance energy due to the thin barrier is very small, and there is no change at all for the  $\delta$ -function potential. The reason for such behavior can be attributed to the nature of the wave function of the second resonance state. A normalized wave function of the first, second and third resonance states with a thin barrier height and width of 65 meV and 15 Å, respectively (upper panel), and with a  $\delta$ -function potential of strength of one eV·Å (lower panel) as an extra potential profile to the RTS, are shown in Fig. 4. As expected, the wave function of the second resonance state vanishes in the middle of the well, and an extra potential profile present in the middle of the well remains unseen by it. Due to the finite width of the thin barrier, the envelop wave function

gets affected over a spatial range, where the small change in resonance energy is a result of such effect. Moreover, the  $\delta$ -function potential is confined to a particular position in spatial dimension and affects only the derivatives of the wave function. If the position of the  $\delta$ -function potential is at a point ( middle of the well) where the wave function of the second resonance state vanishes, then its effect will be absolutely zero on the second resonance state. The results for the third resonance are similar to those of the first resonance due to the similarity in their wave functions, and are not shown here for brevity.

The change in resonance energy and width of the resonance state and the change in density of states  $\Delta N(E)$  at the resonance energy for the first and second resonance states as a function of thin barrier height (15 Å width) and as a function of the strength of the  $\delta$ -function potential at c=0 are shown in Figs. 5 and 6. In Fig. 5, the change in energy of the first resonance state for the symmetric and asymmetric RTS are indistinguishable. Moreover, the increase in the width of the resonance is more pronounced for the asymmetric RTS than the symmetric one. It is clear from earlier discussions (about the width and escape time) that the escape time from a state is less for an asymmetric RTS than from the corresponding state of a symmetric RTS. As we mentioned earlier, the peak value of  $\Delta N(E)$  decreases for a finite height of the thin barrier and finite strength of the  $\delta$ -function potential. This decrease in  $\Delta N(E)$  is correlated with the increase in widths of the resonance states through the quantity  $\Delta N$ [Eq. (4)], but the variation of the width as a function of thin barrier height and strength of the  $\delta$ -function potential in Fig. 5 is entirely different than the variation of  $\Delta N(E)$ . The tails of the Gaussian distribution persist longer for the broader distribution and contribute more to the area of the distribution. Hence, the increase in the width does bring the peak value of  $\Delta N(E)$  down, but the condition  $\Delta N=1$  makes it decrease faster than the increase in the width. The energy of the first resonance state increases exponentially as a function of the thin barrier height and the strength of the  $\delta$ -function potential and approaches the second resonance state. In Fig. 6, as discussed earlier, changes brought about by the thin barrier and  $\delta$ -function potential are negligible. So, the extra potential profile could cause the first resonance state to merge into the second resonance state. The changes in the third resonance state are similar to those in the first one.

#### CONCLUSIONS

In conclusion, we have studied the effect of a scattering center on the transmission and change in density of states for both symmetric and asymmetric resonant tunneling structures by representing it by a thin barrier of variable height and fixed width, and by a  $\delta$ -function potential of variable strength, and placing it in the middle of the well. It is found that because of the extra profile the resonance energies are shifted up, and the widths of the resonance states are increased for the even states. The change in width is the signature of the time-energy uncertainty relation. There are practically no changes in the odd states because of the nature of their wave functions. The peak value of a plot of the change in density of states versus the energy decreases as the height of the thin barrier or the strength of the  $\delta$ -function potential increases. This decrease

is related to the change in the width of the resonance states.

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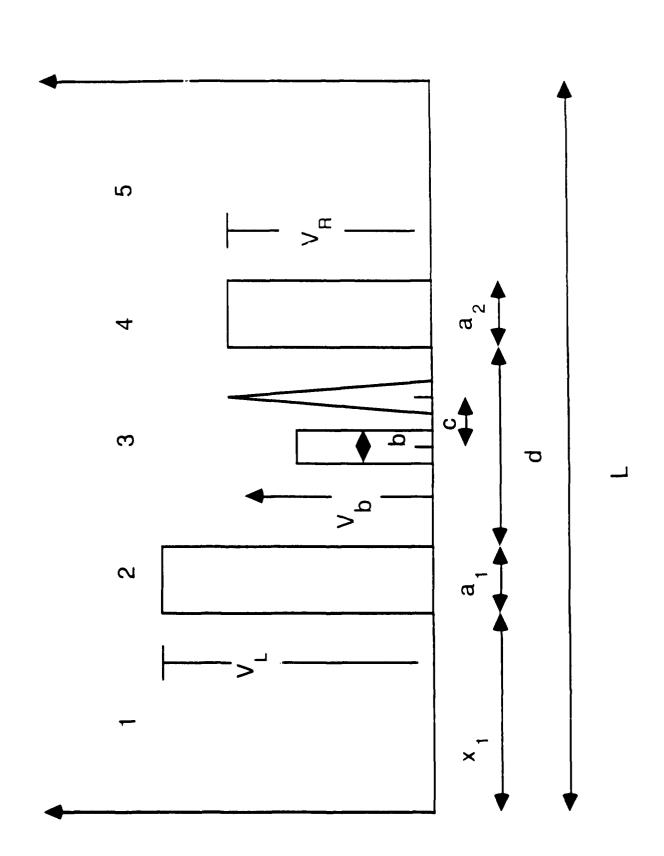
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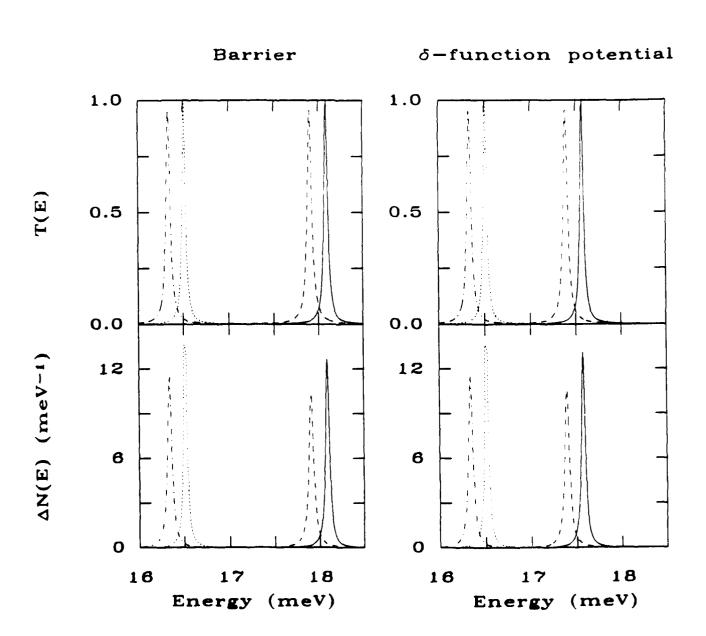
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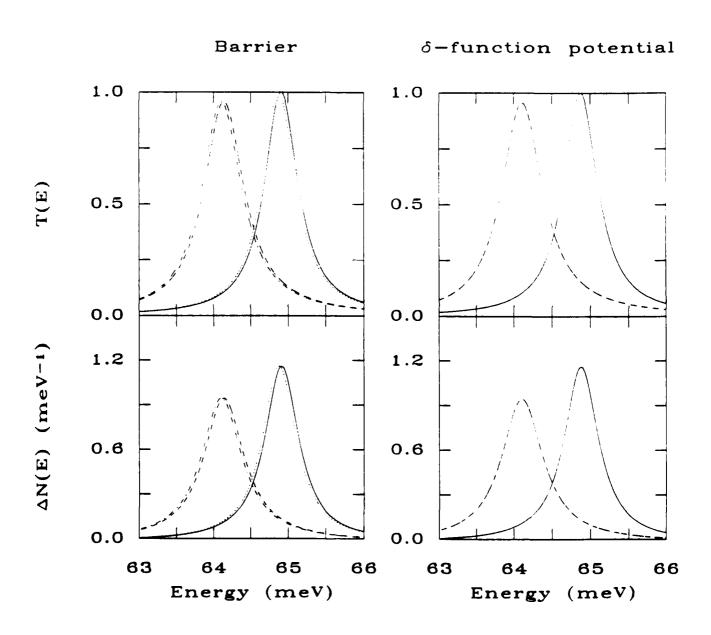
- Fig. 1. Schematic illustration of an asymmetric RTS structure with an extra potential profile in a box. The position of the RTS in the box is  $x_1$  from the left wall. The widths and heights of the two barriers of the RTS are, respectively,  $a_1$  &  $a_2$  and  $V_L$  &  $V_R$ , and the well width is d. A thin barrier of width b and variable height and a  $\delta$ -function potential as shown are considered as an extra potential profile in the RTS.
- Fig. 2. Transmission coefficient T(E) and change in density of states ΔN(E) for a symmetric (solid curve) and asymmetric (dashed curved) RTS with a thin barrier of 15 Å width and 10 meV height and δ-function potential of 100 meV·Å strength, compared with T(E) and ΔN(E) for a symmetric (dotted curve) and asymmetric (dot-dashed curve) RTS with zero thin barrier height and zero δ-function potential strength. The energy range shown is in the neighborhood of the first resonance state.
- Fig. 3. T(E) and  $\Delta N(E)$  for the second resonance state. The different curves are described in Fig. 2.
- Fig. 4. Wave functions of the first (solid curve), second (dashed curve) and third (dotted curve) resonance states for a thin barrier of height 65 meV and width 15 Å( top panel) and a δ-function potential of strength one eV·Å (bottom panel).
- Fig. 5. Change in resonance energy, width of the resonance state and peak value of the ΔN(E) versus E plot of the first resonance state for the symmetric ( solid circles) and asymmetric ( solid triangle) RTS as a

function of thin barrier height (15 Å width) and the strength of  $\delta\text{-function}$  potential.

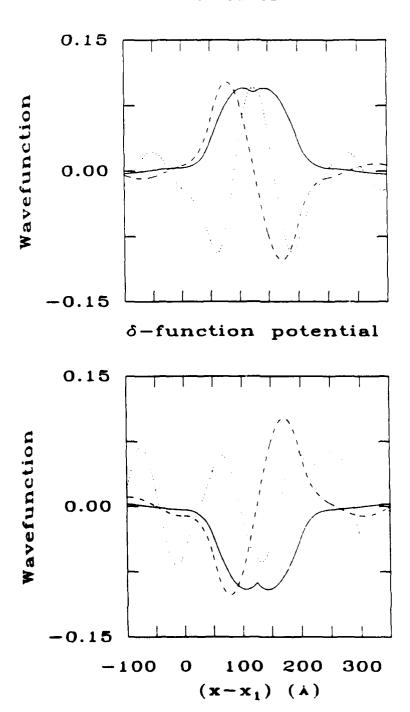
Fig. 6. Same as in Fig. 5 but for the second resonance state.

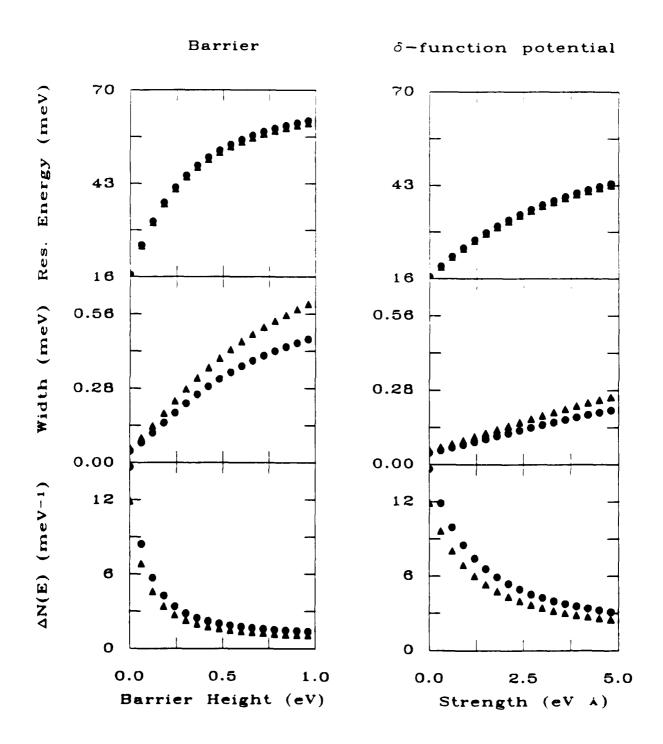


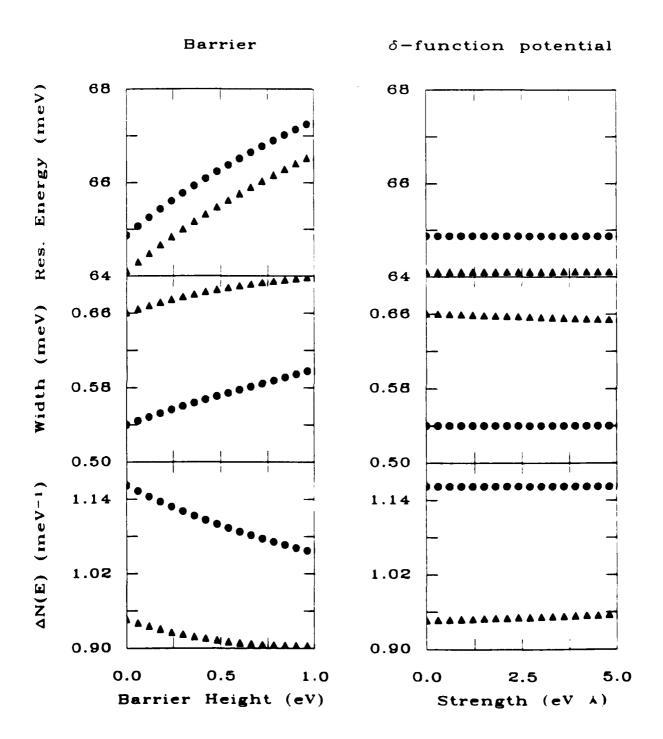












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